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Travelling Turing patterns with anomalous diffusion

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Abstract
We investigate the formation of Turing patterns (arising from a diffusion driven instability) when diffusion is anomalous. We analyse a model that contains the important features of Turing systems and that has been extensively used in the past to model interesting biological patterns. We concentrate on the case of asymmetric anomalous diffusion, and we cast a version of the model, suitable for numerical calculations, using a discrete version of the fractional derivatives defining the anomalous diffusion operator. The results are interesting in the sense that patterns are no longer stationary but acquire a velocity that depends on the exponent of the fractional derivatives. Extensive numerical calculations in one and two dimensions exhibit many of the features predicted by the analysis of the equations.

1. Introduction

There has been a renewed interest in the phenomenon of anomalous diffusion in recent years, mainly due to the fact that it has been proved a useful concept to model many real situations. Anomalous diffusion can be understood by considering a random walk with Levy flights [1]. The important consequence of having a Levy distribution of step lengths that is asymmetric in general, is that the corresponding diffusion equation contains fractional derivatives, instead of the Laplacian operator [2].

It is thought that this situation is realized when diffusion takes place in inhomogeneous or fractal media, therefore there is widespread interest in this phenomenon in many fields of science, including physics [3], biology [4], geology and many more, including complex systems described by non-linear differential equations. Of particular interest are reaction-diffusion systems, which exhibit a diffusion driven instability and that usually give rise to the formation of spatially stable patterns.

The analysis of reaction diffusion equations with fractional derivatives in time has been treated by Henry and Wearne [5]. The conditions for a Turing instability are studied in detail, in one dimension, for the particular case when the mean square displacement $\langle x^2 \rangle \approx t^{1/2}$ (sub diffusion). It is shown that the range of ratios of diffusion coefficients in which a pattern is stabilized widens. This, in itself, is interesting and applicable to Turing systems that take place in inhomogeneous or fractal domains, as is often the case for biological tissues.

Therefore, it is important to investigate the effect of anomalous diffusion using spatial fractional derivatives. This has been discussed by del Castillo-Negrete *et al* [6]. They use a reaction diffusion equation of the Fisher–Kolmogorov type with asymmetric Levy flights. They see that a wavefront with constant velocity in normal diffusion conditions would be accelerated in the case of anomalous diffusion, and that the decay of the front becomes power law.

Furthermore, the direction in which this wavefront travels can be chosen because of the asymmetry of the problem. As pointed out elsewhere [5], it is interesting to study the formation of spatial Turing patterns in higher dimensions. In this work we address exactly this issue, restricting ourselves to study a specific model, used in the past to describe various Turing patterns in nature [7]. The reasons for doing this are manyfold: first, it allows a detailed analysis of the instability [8] and its ranges of appearance in the Turing regime, second, it is straightforward to perform reliable numerical calculations and compare them with the ones obtained in the normal case, and finally, one could discern which of the features of anomalous diffusion could be generalized to other models.

2. The model

Turing equations can be written in general as

$$\frac{\partial \hat{U}}{\partial t} = \mathbf{D}\nabla^2 \hat{U} + F(\hat{U}) \tag{1}$$

where $\hat{U}$ is a vector, whose components are concentrations of chemicals, and $\mathbf{D}$ is a matrix of diffusion coefficients. The non-linear functions F represent the chemical reactions among different species.

Let us concentrate on a specific Turing model with only two chemicals, devised to study generic properties of the Turing instability. This model is obtained by assuming a stable state in the absence of diffusion and Taylor expansion up to cubic terms in the non-linear functions, obeying all the relevant conservation laws between chemicals,

$$\begin{aligned} \frac{\partial u}{\partial t} &= \delta D \nabla^2 u + \alpha u(1 - r_1 v^2) + v(1 - r_2 u) \\ \frac{\partial v}{\partial t} &= \delta \nabla^2 v + v(\beta + \alpha r_1 u v) + u(\gamma + r_2 v). \end{aligned} \tag{2}$$

In the case of anomalous diffusion one has to use, instead of the Laplacian the fractional derivative operator. The Riemann–Liouville definition is

$${}_a\mathsf{D}_x^{\nu} u = \frac{1}{\Gamma(2-\nu)} \partial_x^2 \int_a^x \frac{u(x')}{(x-x')^{\nu-1}} \, \mathrm{d}x' \tag{3}$$

in each of the coordinates where there is anomalous diffusion. That is

$$\nabla^2 \longrightarrow {}_a\mathsf{D}_x^{\nu_x} + {}_b\mathsf{D}_y^{\nu_y} + {}_c\mathsf{D}_z^{\nu_z} \equiv \Delta_\nu^a.$$

In general our model now reads

$$\begin{aligned} \frac{\partial u}{\partial t} &= \delta D \Delta_\nu^a u + \alpha u(1 - r_1 v^2) + v(1 - r_2 u) \\ \frac{\partial v}{\partial t} &= \delta \Delta_\mu^a v + v(\beta + \alpha r_1 u v) + u(\gamma + r_2 v). \end{aligned} \tag{4}$$

An important property of the fractional calculus is that

$$_{-\infty}\mathrm{D}_x^{\nu_x} \mathrm{e}^{\mathrm{i}kx} = (\mathrm{i}k)^{\nu_x} \mathrm{e}^{\mathrm{i}kx}.$$

Therefore, the Fourier transform of the fractional derivative of any function simply gets multiplied by the factor $(\mathrm{i}k)^\nu$.

One can perform a linear analysis to investigate the region of parameter space where the instability takes place. In the absence of diffusion any perturbation has time dependence $\mathrm{e}^{\omega t}$ and stable modes have $\mathrm{Re}(\omega) < 0$. In the presence of diffusion, the spatial dependence of disturbances is of the form $\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}$, and there is a dispersion relation $\omega(k)$, which predicts the conditions in which some modes k are enhanced parametrically, when $\mathrm{Re}(\omega(k)) > 0$. Without loss of generality, one shall set $\gamma = -\alpha$, in order to have single stable state at $(u, v) = (0, 0)$. In one dimension, and when only the concentration field u presents anomalous diffusion ($\mu = 2$), we obtain the following dispersion relation

$$\omega^2 - B\omega + C = 0$$

where

$$\begin{aligned} B &= -\alpha - \beta + \delta k^2 - \delta D(\mathrm{i}k)^\nu \\ C &= \alpha\beta + \alpha(1 - \delta k^2) + \delta D(\beta(\mathrm{i}k)^\nu - \delta(\mathrm{i}k)^\nu k^2). \end{aligned} \tag{5}$$

As usual, for a choice of parameters, one can fulfil the conditions for a Turing instability. In this case the modes with $\mathrm{Re}(\omega) > 0$ must have a non-zero imaginary part, as seen in equation (5). This means that the parametrically enhanced modes should oscillate in time. This oscillation is different to the one observed in a true Hopf bifurcation (which our model also presents when $\beta < -1$) [8], in that the asymmetry of the imaginary part of $\omega(k)$ produces a travelling wave, instead of a stationary oscillating pattern.

In the case of asymmetric anomalous diffusion, if a Turing pattern is finally stabilized by the non-linear terms, the concentrations of morphogens need to oscillate at each point of space. In fact, we shall demonstrate that this imaginary part produces a wavefront that travels at constant velocity in d-dimensions, in a direction given by the anomalous diffusion parameters (ν_i). In general, one could investigate numerically the limits of the region for which $\mathrm{Re}(\omega) > 0$ by letting $\omega \to 0$ in the transcendental equation (5).

In the special case when $\nu = 1$, the maximum of $\mathrm{Re}(\omega)$ is found when $k \to \infty$. Then, the dispersion relation reads, approximately,

$$\omega^2 - \omega D\delta \mathrm{i}k - D\delta \mathrm{i}k^3 - \alpha k^2 = 0,$$

or, in general

$$\omega \sim \alpha + D\delta \mathrm{i}k. \tag{6}$$

It is seen that there is a parametric enhancement of modes with very short wavelength and there is a travelling wave with phase velocity given by $c = D\delta$.

Alternatively, one could use equation (5) and find numerically the wavevector $k_{\max}$ where $\mathrm{Re}(\omega)$ is maximum, and defining a phase velocity as

$$c = \frac{\mathrm{Im}[\omega(k_{\max})]}{k_{\max}}.$$

In figure 1 we show the results of doing exactly this numerical exercise. In all the numerical calculations presented in this paper we fix $\alpha = 0.899$, $\beta = -0.91$, $\gamma = -\alpha$ and $D = 0.416$. This ensures that one is well into the region where a Turing instability appears [8].

Observe that the maximum velocity is found at a point larger than $\nu = 1$. Also, as expected, when $\nu = 2$ the velocity is zero, and we recover the stationary patterns. For super diffusion

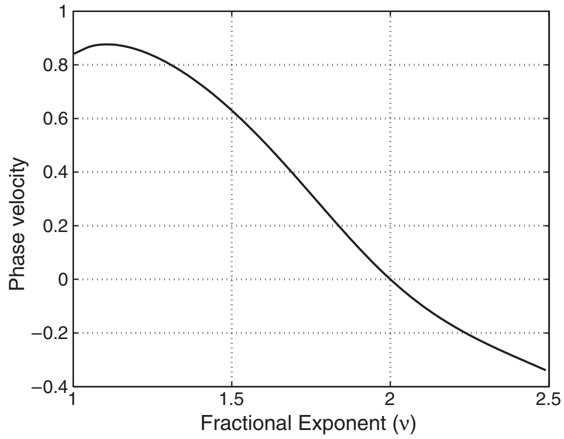

Figure 1. Wavefront phase velocity as a function of the fractional exponent for anomalous diffusion ν.

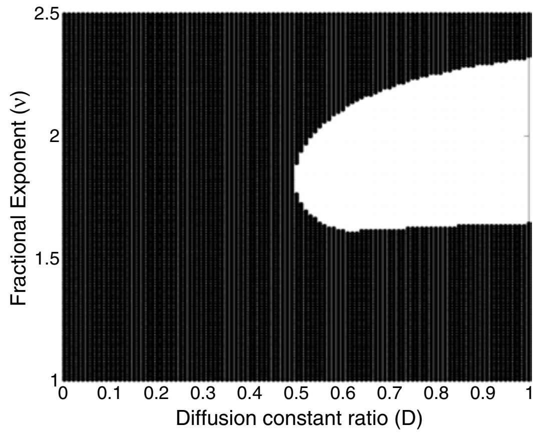

Figure 2. The shaded area in parameter space for which $\mathrm{Re}(\omega) > 0$.

$\nu > 2$ the velocity is reversed. The direction in which the wavefront travels is determined by the choice of the sign of k, which is arbitrary and reflects the asymmetry imposed in the problem.

We also investigated numerically the region of the parameter space (ν, D) where $\mathrm{Re}(\omega) > 0$. As conjectured in [5] the range of values of the ratio of diffusion constants (D) for which there is a possible Turing instability is widened by anomalous diffusion. In figure 2 we show this region as a shaded area. Notice that very near $\nu = 2$ the range is expanded for super diffusion and contracted for sub diffusion. Also notice that there is a situation of reentrant instability around $\nu = 1.63$. For smaller ν there are always patterns, but we cannot ensure that all of them are stabilized. In fact we know that for $\nu = 1$ they are not.

3. Numerical patterns

We performed numerical integration of equation (4) by using a simple Euler method, described elsewhere [7]. The only difference is that instead of the discrete Laplacian in a grid, we have to calculate a discrete fractional derivative. We used the so called Grundwald–Letnikov form [9] of the Riemann–Liouville standard definition. This is,

$$\Delta_\nu^1 u(n) = \sum_{j=0}^{n-1} (-1)^j \binom{\nu}{j} u(n-j) \tag{7}$$

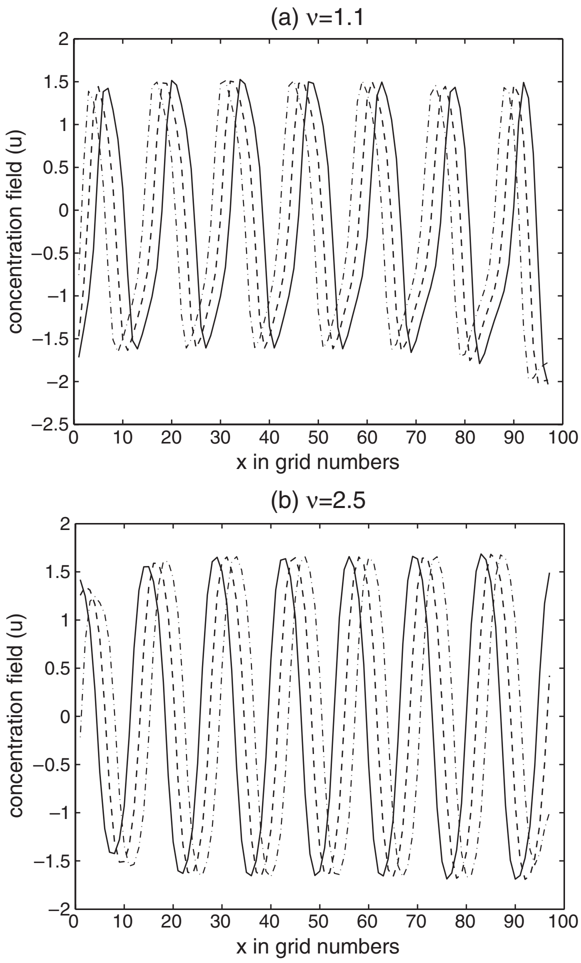

Figure 3. (a) One dimensional numerical pattern obtained when $\nu = 1.1$. The whole pattern travels to the left: the initial time is shown as a full curve, then after 700 time steps one gets the dashed curve and after a further 700 steps one gets the dashed–dot curve. (b) The same as (a) but for $\nu = 2.5$. The time intervals are 2000 in this case, and the pattern travels to the right.

where the grid has N intervals, such that $n \in [1, N]$ is an integer that gives the position in units of the grid. This form tends to equation (3) in the limit when the variable becomes continuous (an infinitely fine grid) and gives the correct expression for the discrete Laplacian when ν is 2.

We impose periodic boundary conditions by extending the grid by two on both extremes of the domain and demanding that

$$u(N+1) = u(1); \qquad u(N+2) = u(2);$$
$$u(0) = u(N); \qquad u(1) = u(N-1).$$

The combinatorial coefficients were calculated with a numerical Euler gamma function. The calculations in one dimension corroborate the predictions of linear analysis.

In figure 3 we show the spatial patterns stabilized for two different values of ν while keeping $\mu = 2$. The snapshots shown at different times illustrate the fact that the pattern travels in one direction for sub diffusion and in the opposite direction for super diffusion. Notice that the wave shape in (a) is quite complicated, reflecting the complexity of the dispersion relation and the presence of many modes.

In figure 4 we show the fast Fourier transforms patterns with (a) $\nu = 2$ and (b) $\nu = 1.01$ for comparison. Observe that the Laplacian case (normal diffusion) displays an almost

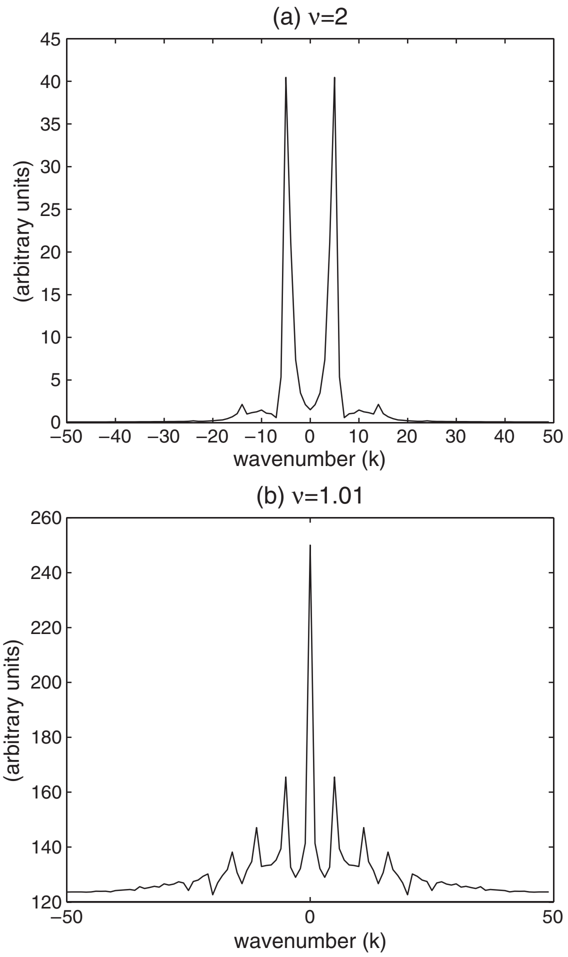

Figure 4. (a) Fast Fourier transform of a one dimensional pattern obtained with normal diffusion $\nu = 2$. (b) The same as (a) but for $\nu = 1.01$.

monochromatic wave, resulting in a practically pure sinusoidal wave shape, while the sub diffusive case shows many peaks and tails that extend to very large wavenumbers.

In two dimensional planes, calculations were performed in the same way by defining a square grid. In these calculations we kept $\nu_x = \mu_x$ and $\nu_y = \mu_y$. It is seen that once a Turing pattern is stabilized, it travels in the proper direction, at an angle proportional to $\tan^{-1}(\nu_y/\nu_x)$.

In figure 5 a pattern of spots, obtained with $r_1 = 0.02$ and $r_2 = 0.2$, and $\nu_i = \mu_i = 1.8$ is shown in consecutive times. The size of the grid is 48×48, and the scale of the pattern is given by $\delta = 2$. The pattern in figure 5 is not fully converged, since it has a conspicuous defect. In the case of normal diffusion this defect would take a very long time to heal (in large systems the number of defects decreases following a power law with time), but with anomalous diffusion healing of defects is very efficient. Converged patterns are always defectless.

We also obtained patterns with stripes, by choosing $r_1 = 0.35$ and $r_2 = 0.02$. It is seen that the stripes always align themselves perpendicular to the direction of motion, as it is illustrated in figure 6 where one can observe that the pattern travels exactly towards the bottom left corner, since both fractional exponents are the same. It is also very clear that while travelling the pattern heals defects very easily, and eventually becomes defectless.

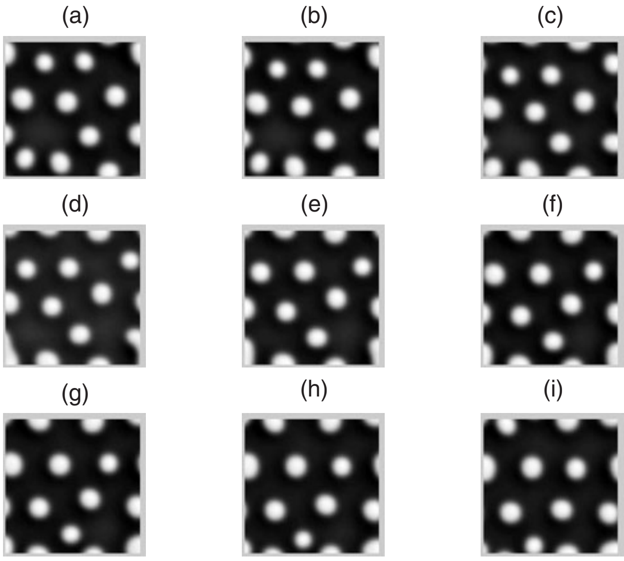

Figure 5. Nine snapshots in alphabetic sequence of a Turing pattern with sub diffusion. The time interval between each picture is 5600 time steps. Observe that the pattern travels towards the lower left corner and that the spots are rearranged while travelling.

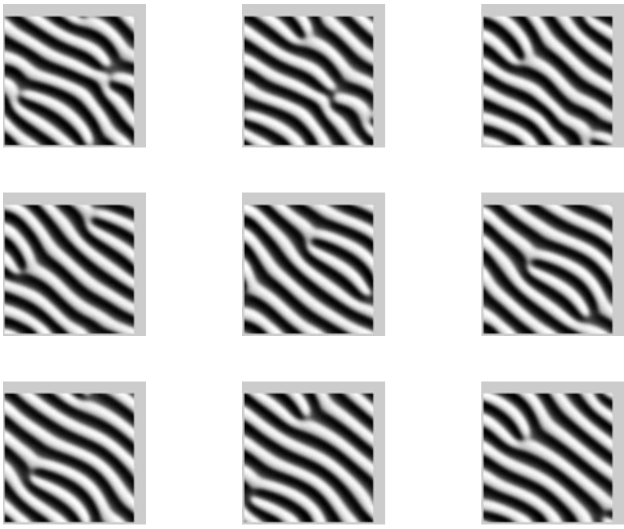

Figure 6. Two dimensional pattern obtained with non-linear parameters appropriate for stripes. The values of the fractional exponents were all equal $\nu_i = \mu_i = 1.5$. We show snapshots separated by 5600 time steps, and ordered as in figure 5.

The fact that the stripes are always perpendicular to the direction of motion can be used to orient the patterns to any given direction by just changing the ratio of fractional exponents. This is shown in figure 7, where the formation of a pattern with $\nu = 1.5$ and $\mu = 1.2$ is followed every 5600 time steps. The initial conditions are random in a square region in the centre of the domain and zero elsewhere. These initial conditions were tried to verify that the final pattern does not depend on them. Notice how rapidly the instability settles down, and the robustness of the rolls in a different orientation than the 45° shown in figure 6.

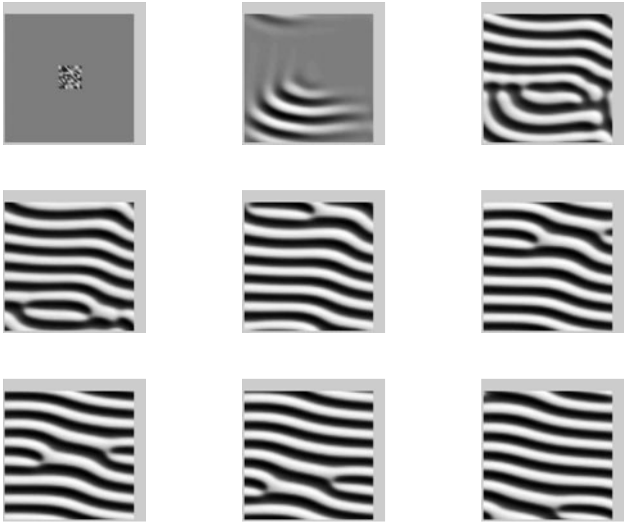

Figure 7. Same as figure 6, except that the values of the fractional exponents were $\nu_i = 1.5$, and $\mu_i = 1.2$. We show snapshots separated by 5600 time steps, starting from the initial conditions.

There are some situations in which the orientation of patterns is important. For instance, the stripes on the coat of a baby Angel fish *Pomacanthus imperator* are semicircular and mostly oriented vertically. When the fish grows to an adult state, the stripes become horizontal. In general there are dislocation like defects, different on either side of the fish, and it is observed that these dislocations tend to disappear with time. The transition takes only a few weeks, and a sort of square pattern that starts with fine horizontal needles stemming from the vertical stripes is observed. We performed a simple numerical calculation to see the kind of orientation transition that is forced when one changes the anisotropy of the anomalous diffusion.

In figure 8 we first converged a defectless horizontal pattern by setting $\nu = 2$ and $\mu = 1.18$. Then we suddenly change to $\nu = 1.18$ and $\mu = 2$, in order to force a vertical pattern. Observe the transitory patterns that appear very rapidly, mimicking the patterns observed in the fish. In a former study [10], we used the present Turing model with normal diffusion to simulate the coat of the fish, defining a domain with the approximate shape of the animal. The problem was to correctly orient the pattern with zero flux boundary conditions. To achieve this we imposed a field in one of the boundaries to keep the concentration fixed at this border. We called this a source of morphogens. As we see here, there is an easier and more realistic way of orienting the patterns by simply considering that the homogeneity properties of the tissue where the morphogens diffuse and change as the fish grows. Further work is needed to test this idea.

To conclude this section we show an interesting calculation performed in a spherical domain. For this we need to apply the equivalent of the Laplacian operator in spherical coordinates to the case of fractional derivatives. The general expression for the diffusion operator in curved and growing domains has been given in [12], and for a steady spherical surface it is

$$\frac{1}{r^2 \sin(\theta)} \frac{\partial}{\partial \theta} \left(\sin(\theta) \frac{\partial u}{\partial \theta} \right) + \frac{1}{r^2 \sin(\theta)} \frac{\partial^2 u}{\partial^2 \phi}.$$

One defines a grid in the angular variables $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$, and makes a discrete convolution, as the one in equation (7), in the azimuthal variable ϕ, resulting in a fractional differential operator instead of the second derivative with respect to ϕ. Care has to be taken

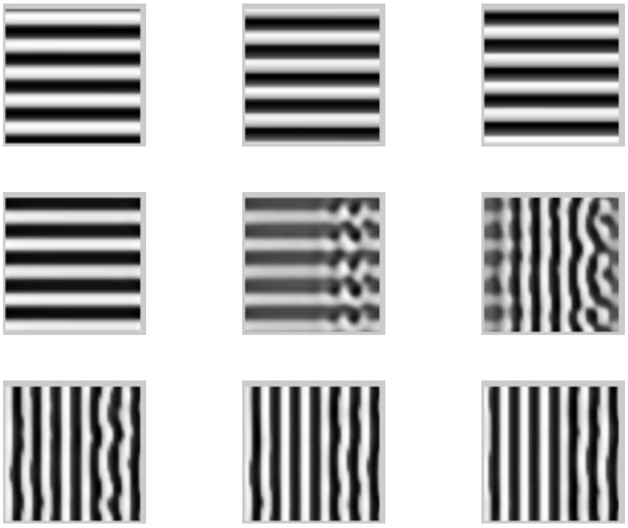

Figure 8. Snapshots of a Turing pattern during a transition from horizontal to vertical stable stripes. The sequence is as usual.

Figure 9. Nine snapshots, s in figure 5, of a Turing stripe pattern on a sphere. The pattern revolves clockwise and a spiral vortex is formed at each pole due to the different angular velocity. The position of the poles is given by the values of the fractional exponents.

to correctly define periodic boundary conditions at $\phi = 0$ and 2π. In θ, periodic conditions are attained by connecting each point to the corresponding point at a distance $\pi - \delta\theta$. This procedure is explained in detail elsewhere [11]. The results are shown in figure 9 for the case when $r_1 = 3.5$, $r_2 = 0.02$, $\nu_i = 2$, $\mu_\theta = 2$ and $\mu_\phi = 1.2$. It is found that once the stripes converge, only two major defects appear at the poles, given by the direction of rotation imposed by the values of the fractional exponents (not the origin of the coordinates). The velocity of rotation diminishes as one leaves the poles, producing a sort of spiral vortex. The stripes are continuously exchanging dislocations to cope with this dynamics, as clearly observed in the last three frames.

4. Conclusions

In this paper we have explored the formation of patterns in Turing systems when diffusion is anomalous. We conclude that in general the parametrically enhanced modes have complex roots, and oscillating patterns with wavefronts are formed. In the case of asymmetrical diffusion, travelling waves are present in the pattern. It was shown that super diffusion widens up the range of ratios of diffusion coefficients that meet the Turing conditions for instability. Another important feature predicted by the model and numerical calculations is that striped patterns can be oriented and that the defects are very effectively suppressed. These two facts may be extremely important in applications to biological systems, for instance, the stripes of the baby fish *Pomacanthus imperator* change orientation when the fish attains adulthood, and at present we are pursuing the possibility of invoking anomalous diffusion to explain this phenomenon.

Numerical calculations also show that the wave shape is very complicated, as compared to the case of normal diffusion, due to the fact that many more modes are enhanced by the instability. This opens up a lot of possibilities to explain complicated patterns exhibited by many animals with simple Turing mechanisms. We expect that these results could be translated to other models in which diffusion is present, in particular equations of the Landau–Ginzburg type. We have the knowledge that the Fisher–Kolmogorov equation studied in [6] exhibits the same features.

Also important for applications is the behaviour of the pattern revealed by our numerical calculations on a sphere with anomalous diffusion, in the case of striped patterns, the spiralling observed is very interesting and could be applied to systems in which a coherent motion is needed, as in the heart [4]. In the case of spotted patterns on a sphere, it has been shown that they provide good models for the shape of viruses, where the symmetry of the spots is basically governed by the radius of the sphere. The patterns with anomalous diffusion would help to get rid of unwanted defects and attain the observed symmetry very easily.

Further research is needed to corroborate if anomalous diffusion is an important feature in a real system. Some beautiful experiments preparing systems with Levy flights have been performed [1], we need the same experimental ideas in the case of diffusion driven pattern formation.

Acknowledgments

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References

[1] Solomon T H, Wooks E R and Swinney H L 1993 *Phys. Rev. Lett.* **71** 3975
[2] Zanette D H 1997 *Phys. Rev.* E **55** 1181
[3] Gentle K W *et al* 1995 *Phys. Plasmas* **2** 2292
[4] Winfree A T 1997 *Int. J. Bifur. Chaos Appl. Sci. Eng.* **7** 487
[5] Henry B I and Wearne S L 2002 *SIAM J. Appl. Math.* **62** 870
[6] del Castillo-Negrete D, Carreras B A and Lynch V E 2003 *Phys. Rev. Lett.* **91** 018302
[7] Barrio R A, Varea C, Aragón J L and Maini P K 1999 *Bull. Math. Biol.* **61** 483
[8] Leppänen T, Karttunen M, Barrio R A and Kaski K 2004 *Phys. Rev.* E at press
[9] Podlubny I 1999 *Fractional Differential Equations* (San Diego, CA: Academic)
[10] Aragón J L, Varea C, Barrio R A and Maini P K 1998 *FORMA* **13** 154
[11] Varea C, Aragón J L and Barrio R A 2000 *Phys. Rev.* E **60** 4588
[12] Sánchez Garduño F and Barrio R A 2004 *Growth, Curvature and Patterns: The Influence of the Domain Dynamics into Patterning* (Singapore: World Scientific) at press